

Tetrachloroethylene-13C1
287399-46-6 | DTXSID30481626

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.29e-13 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.63e-01

Confidence level: 6.35e-01

Nearest Neighbors from the Training Set

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Tetrachloroethylene

Measured: 1.67e-13

Predicted: 2.29e-13

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Trichloroethylene

Measured: 2.36e-12

Predicted: 2.21e-12

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Chloral

Measured: 1.60e-12

Predicted: 1.64e-12

Image not found

Oxazole

Measured: 9.10e-12

Predicted: 3.15e-11